CCSI

Carbon Capture Simulation Initiative

Overview for RUA Meeting

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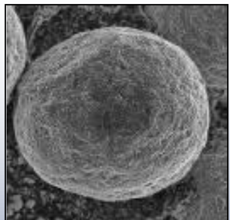
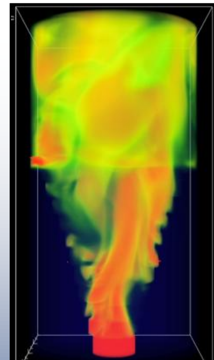
5 March 2013

CCSI: Accelerating Technology Development






Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

National Labs

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Pacific Northwest National Laboratory
NETL
Los Alamos National Laboratory EST. 1943
Lawrence Livermore National Laboratory

Academia

Carnegie Mellon
Princeton University
West Virginia University
Boston University
The University of Texas at Austin
Institute for Clean and Secure Energy, The University of Utah

Industry

Fluor
ADA Environmental Solutions
B&W the babcock & wilcox company
GE
EPRI Electric Power Research Institute
Air Products
Burns & McDonnell Since 1898
Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
Alstom
Southern Company
Duke Energy
URS
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Eastman

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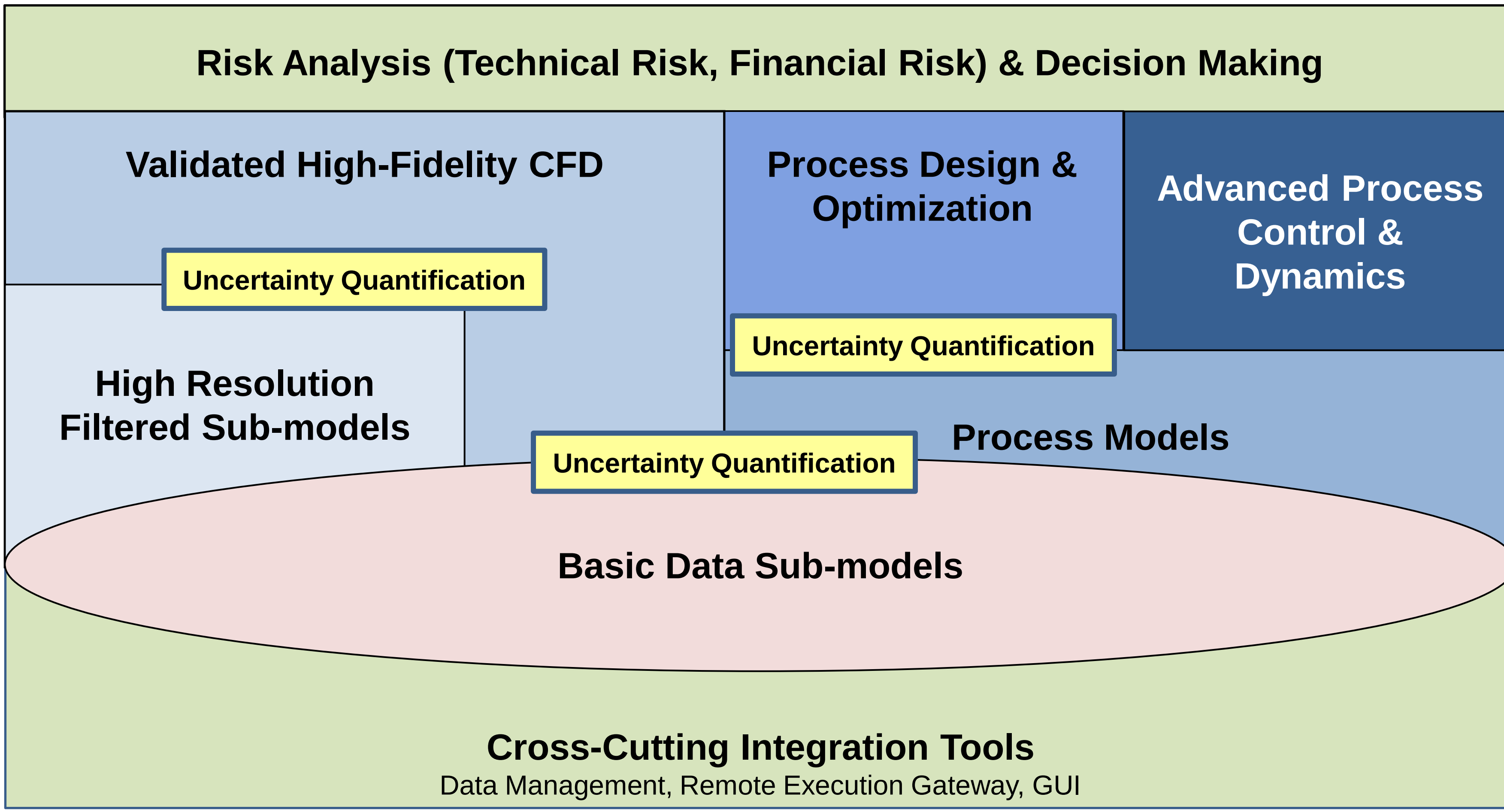
Computational Tools to Accelerate Next Generation Technology Development



CCSI Carbon Capture Simulation Initiative

NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · U.S. Department of Energy

CCSI Timeline

- Organizational Meetings
  - March 2010 - October 2010
- HQ organized Scientific Peer Review: Jan 25, 2011
- Technical work initiated: Feb. 1, 2011
- Industry Advisory Board (IAB) Workshops
  - Feb. 2011 (Berkeley, CA)
  - Sept. 2011 (Morgantown, WV)
- Board of Directors Review: January 2012
- IAB Workshop: April 2012 (Washington, DC)
- SCC Merit Review (ASME): April 2012 (results received Oct. 2012)
- Preliminary Release of CCSI Toolset: September 2012
- Industry Advisory Board Workshop: Oct. 2012 (San Francisco, CA)
- Technical Team Planning: Dec. 2012
- CCSI Year 3 begins: Feb. 1, 2013
- Industry Advisory Board Workshop: April 2013 (Reston, VA)

8 Product Teams

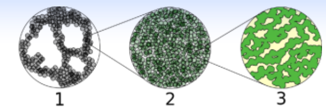
Product categories: organize toolset based on components

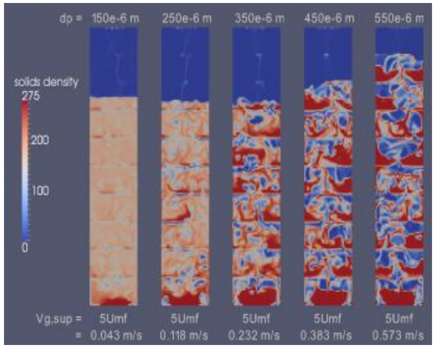
1. Basic data submodels (Joel Kress)
2. High resolution filtered submodels (S. Sundaresan/X. Sun)
3. Validated high-fidelity CFD models & UQ tools (X. Sun/C. Storlie)
4. Process models (D. Bhattacharyya/D. Miller)
5. Process optimization & UQ (D. Miller/C. Tong)
6. Integrated framework for dynamics & control (S. Zitney)
7. Risk analysis & decision-making (C. Dale/D. Engel)
8. Crosscutting integration tools (D. Agarwal)

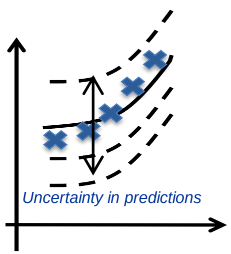
CCSI Deploys Initial Computational Toolset

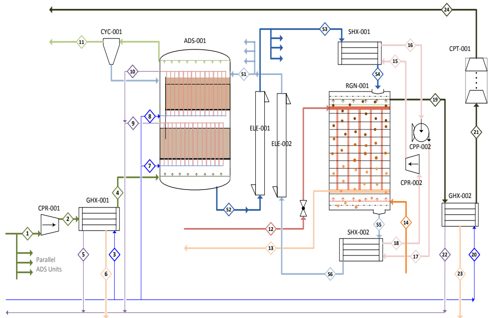
Carbon Capture Simulation Initiative

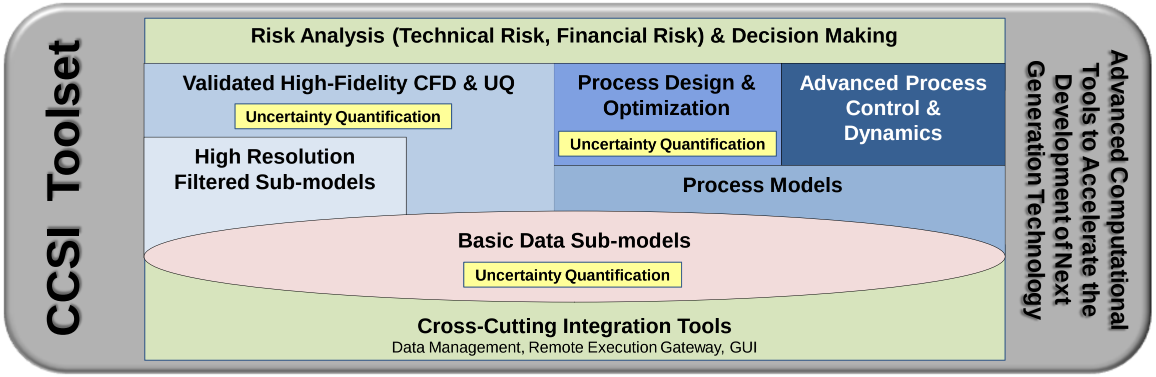
- Released 21 Toolset components Sept. 2012
  - Reaction kinetics model of solid sorbents
  - CFD models of 1 MW adsorber & regenerator
  - Process models of solid-sorbent capture, membrane, and compression systems
  - New optimization tools (ALAMO, superstructure, framework)
  - Advanced dynamic & control models (adsorber, compression
  - New integration tools (REVEAL, Turbine, Sinter)
  - Uncertainty Quantification Framework
  - Financial Risk Tool

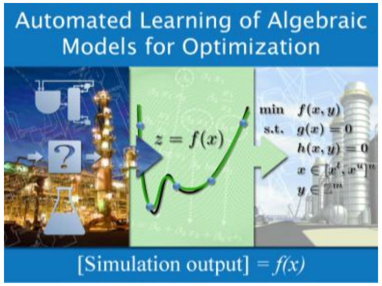


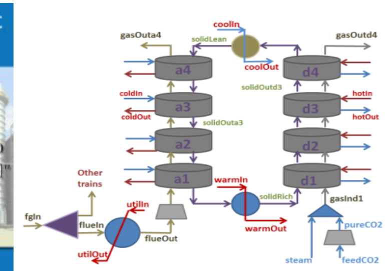












Carnegie Mellon | West Virginia University | Princeton University | Boston University

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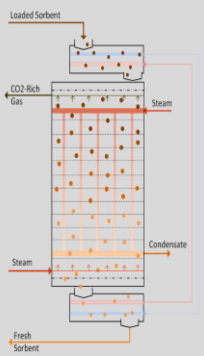
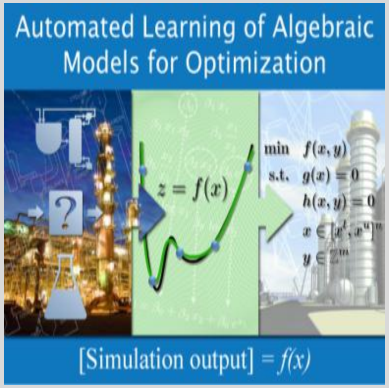
Methodology for determining optimal process configurations

Process Models



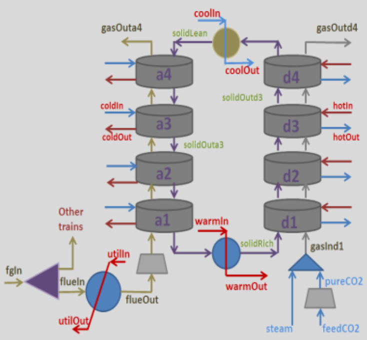
Develop detailed models of major equipment in commercial process simulation tools

Algebraic Surrogate Models



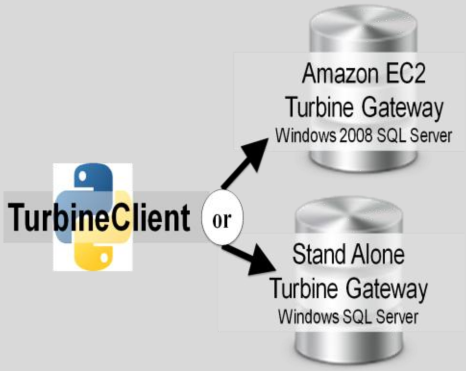
Convert detailed process models to algebraic models for optimization

Superstructure Optimization



Formulate and solve superstructure to determine optimal process configuration

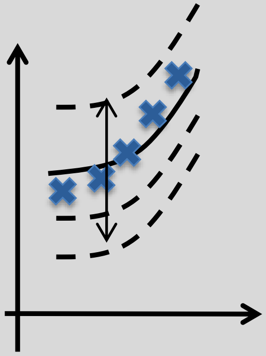
Simulation Gateway



Develop detailed process design based on optimal process configuration

Refine optimal process using detailed process models

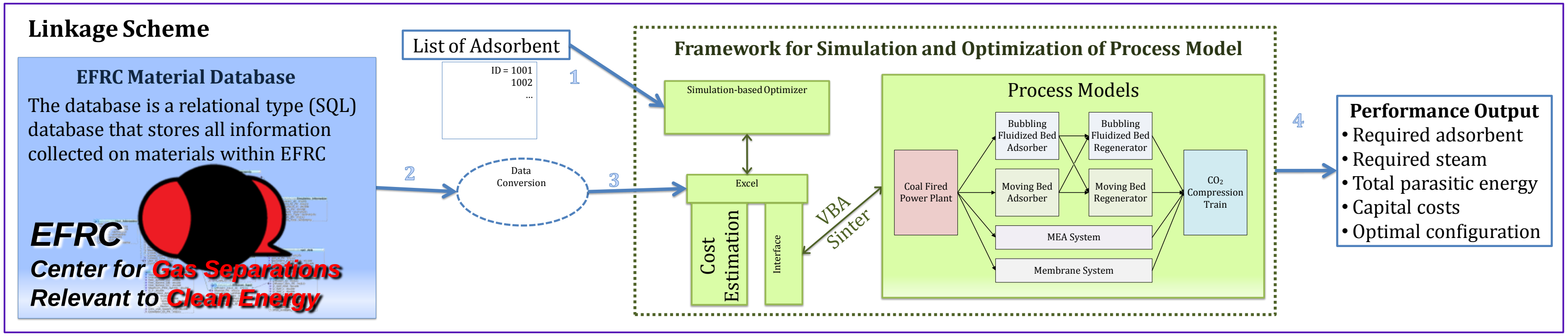
Uncertainty Quantification



Quantify uncertainty in model predictions

Identifying promising concepts more quickly

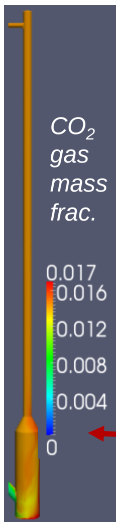
- **How?**
  - Computationally screen sorbent materials, devices, and processes
  - Determine optimal processes for screening & initial analysis
- **CCSI Examples**
  - Simulation-based optimization tools to design optimal capture process
  - Toolset linked to database developed by UC Berkeley Energy Frontier Research Center (EFRC)
    - EFRC database contains over 100,000 zeolite and zeolitic imidazolate framework (ZIF) sorbent structures1
- **Benefits**
  - Optimal process design enables a screening based on best possible conditions customized for specific material properties, ensuring assessment of the full potential of a technology
  - By identifying promising concepts early, time and money are saved because the development efforts are only directed toward potentially successful systems

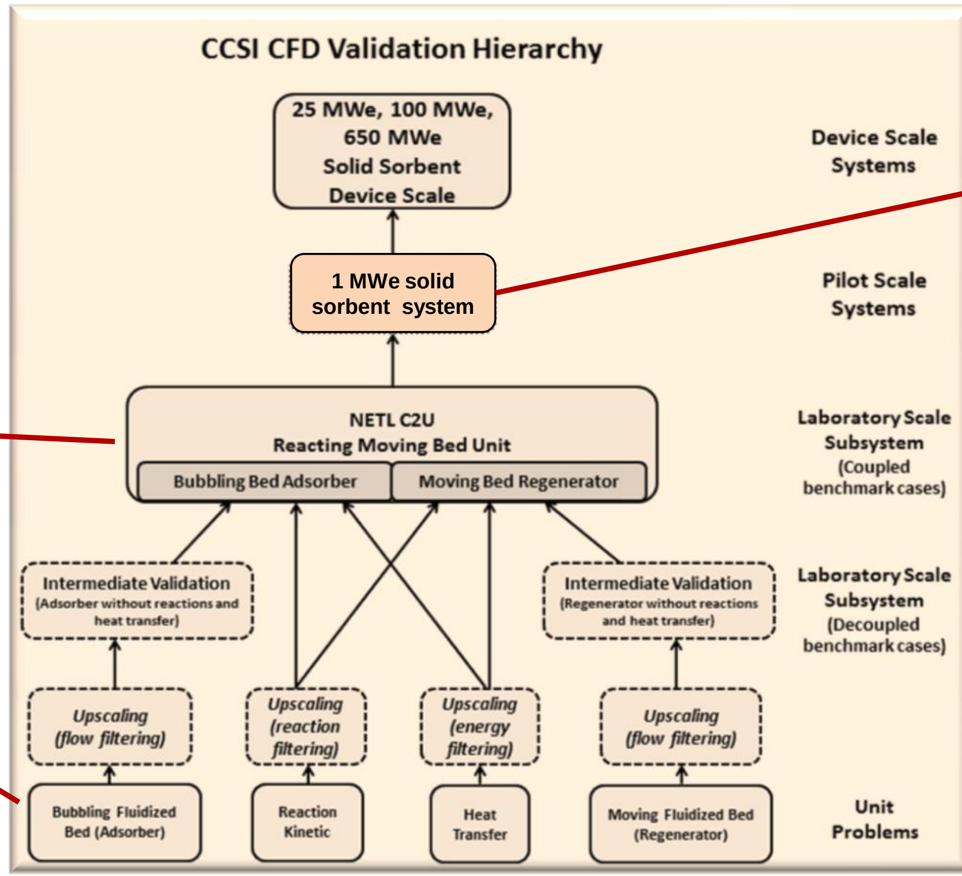


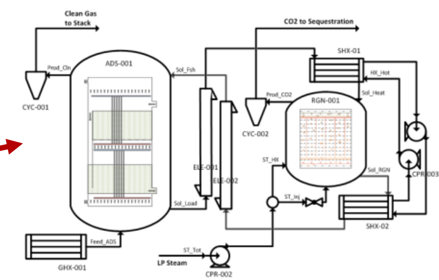
1. L.-C. Lin … B. Smit, In silico screening of carbon-capture materials, *Nat Mater* **11** (7), 633 (2012)

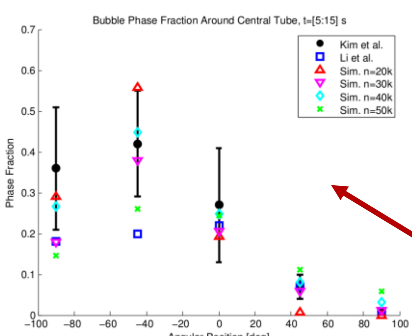
Establishing confidence in the predictions: Validation/Uncertainty Quantification

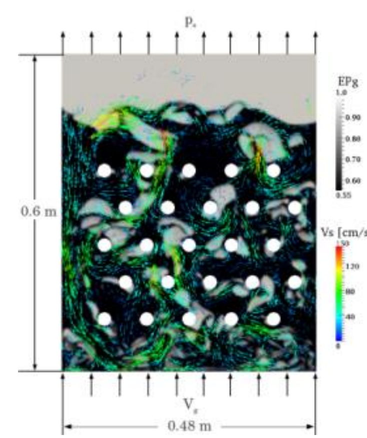
Objective: To provide quantitative confidence on device-scale (CFD) model predictions for devices that are yet to be built.











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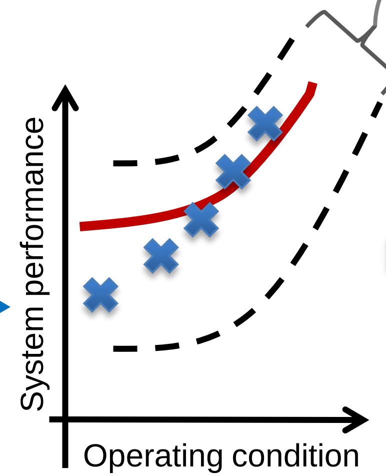
Uncertainty Quantification: How certain are we that our model can predict the system performance accurately?

- How to quantify these error bounds *a priori*?
- How to reduce these bounds?

Scaled-up design

CCSI simulation

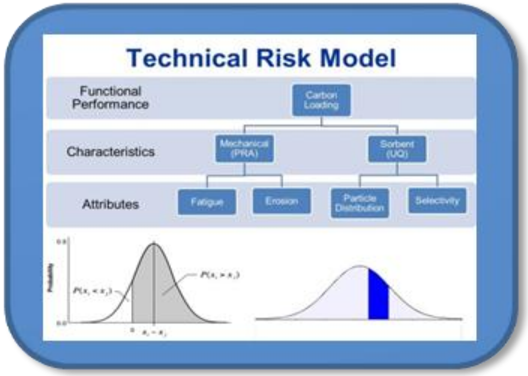


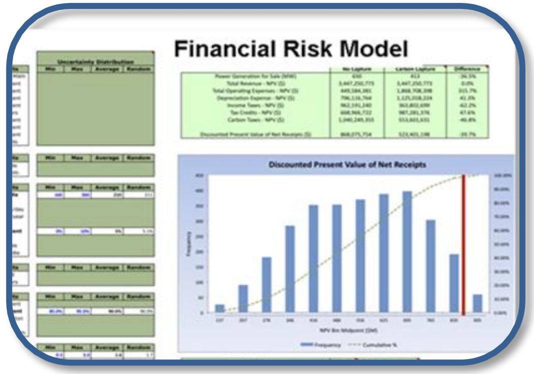
Risk analysis

How does the uncertainty in the prediction affect the risk assessment outcome?

Risk analysis and decision making framework

Combine technical risk and financial risk factors into an integrated decision analysis framework that naturally handles propagation of uncertainties into a variety of decision metrics.

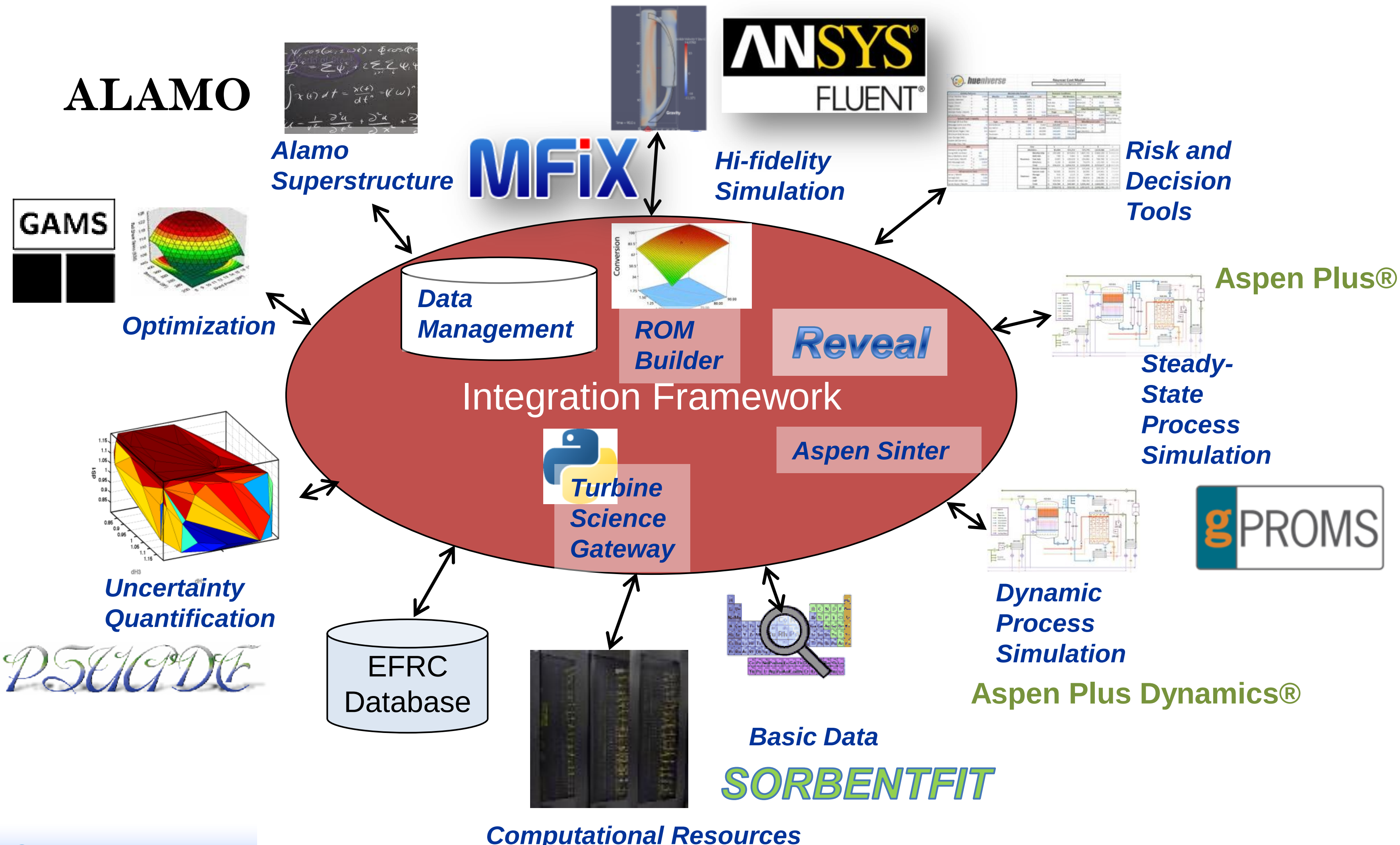




Technical Risk Analysis

Financial Risk Analysis

CCSI framework for integrating modeling and simulation tools



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